Extended Abstracts of the 2002 International Conference on Solid State Devices and Materials, Nagoya, 2002, pp. 492-493

P4-12

Quantum Chemical Molecular Dynamics Simulation on the Dynamics and Stability of the MgO Protecting Layer in Plasma Display

Momoji Kubo[1], Katsumi Sasata[1], Toshiyuki Yokosuka[1], Tomonori Kusagaya[1], Seiichi Takami[1], Akira Kato[2], Akira Imamura[3], and Akira Miyamoto[1,4]

[1]Department of Materials Chemistry, Graduate School of Engineering, Tohoku University, Aoba-yama 07, Sendai 980-8579, Japan.
Phone: +81-22-217-7235, Fax: +81-22-217-7235, E-mail: momoji@aki.che.tohoku.ac.jp

[2]Hitachi Research Laboratory, Hitachi Ltd., Omika 7-1-1, Hitachi, Ibaraki 319-1292, Japan.

[3]Hiroshima Kokusai Gakuin University, Nakano 6-20-1, Aki-ku, Hiroshima 739-0321, Japan.

[4]New Industry Creation Hatchery Center, Tohoku University, Aoba-yama 04, Sendai 980-8579, Japan.

1. Introduction

Plasma display panel (PDP) has gained much attention for a high definition TV, since it is a flat, thin, and large-size display. PDP has been already commercialized for public and individual use. However, in spite of many experimental efforts, the display performances are still unsatisfactory and the lifetime of the PDP is one of the main unsatisfactory performances. Sputtering of the protecting layer by the energetic plasma particles during the discharge process is one of the important factors that limit the lifetime of the PDP. Hence, MgO thin film is regularly used for the protecting layer in the PDP because of its high anti-sputtering and secondary electron emission abilities [1-3].

The sputtering of the MgO protecting layer in the PDP is caused by the attack of the energetic plasma particles. Moreover, experimentally it is pointed that the electric charges accumulated in the MgO surface also degrade the protecting layer under the plasma condition. However, the experimental observation of the above effect is very difficult and the theoretical analysis is strongly demanded. Especially, the information on the effect of the surface orientation of the MgO protecting layer, such as (001), (011), and (111), is strongly desired, since this information suggests the best MgO surface structure having low sputtering yield.

Hence, we applied our accelerated quantum chemical molecular dynamics program Colors to the dynamic behaviors of the MgO surface under the electric field conditions to investigate the MgO surface stability depending on the surface orientations. Especially, since previously there is no program which can simulate the electric field condition considering both the dynamics and electronic states, we developed a new program for the present purpose in this study.

2. Development of New Simulation Program

Recently, we have succeeded in the development of an accelerated quantum chemical molecular dynamics program Colors based on our original tight-binding theory. Since the above program is more than 5000 times faster than the regular first-principles molecular dynamics program, it can perform long-time simulation with the large system. The validity and applicability of the above program were already confirmed in the various topics [4-5]. In the present study, we modify the above accelerated quantum chemical molecular dynamics program Colors in order to consider the electric fields in the dynamics simulations.

3. Results and Discussion

We investigated the dynamics of the three different MgO surfaces, (001), (011) and (111) under 0.1, 0.15, 0.2, and 0.3 V/Å electric fields. Previously, we performed the crystal growth simulation of the MgO(111) surface and clarified that MgO(111) surface is not flat and has quantum dot structure covered by (001) and (011) surfaces. Hence in the present study, as a MgO(111) model we employed the quantum dot structure with (111) orientation covered by (001) surfaces.

Fig. 1 shows the dynamics of the MgO(001) surface at 0.15 V/Å. We can observe that the oxygen atom of the topmost surface is pulled up compared to the Mg atoms, which is caused by the electric field. This result indicates that our program can simulate the effect of the electric field condition to the stability of the MgO protecting layer. Fig. 2(a) shows the final structure of the MgO(001) surface at 0.2 V/Å after the simulation. The vaporization of the oxygen atom from the MgO(001) surface is observed. This result indicates that the electric charges accumulated in the MgO surface degrade

the MgO protecting layer, which confirms the experimental prediction on the effect of the accumulated charges on the surface stability. Fig. 2(b) shows the final structure of the MgO(001) surface at 0.3 V/Å. The evaporation of a large MgO cluster is observed. It indicates that a large accumulated electric fields significantly degrade the MgO protecting layer.

Table 1 shows the effect of the orientation of the MgO surfaces on the vaporization of the atoms or clusters of the MgO surface. In this table, "not" means that the evaporation of the atoms or clusters was not detected, while "evap." means that the evaporation of atoms or clusters was detected. These results indicate that the surface orientation greatly influences the stability of the MgO surface and that the MgO(011) surface has lowest stability and the MgO(111) surface has highest stability.

It is experimentally well known that the MgO(111) surface has lowest stability among (001), (011), and (111) surfaces, which is against our present results. However, our MgO(111) model is not real (111) surface. It has quantum dot structure with (111) orientation covered by (001) surfaces. Hence, we suggests that MgO quantum dot structure with (111) orientation covered by (001) surfaces has the highest stability compared to MgO(001) and MgO(011) surfaces.

4. Conclusion

Our new program enables us to clarify the effect of the electric fields on the stability of the MgO protecting layer in the PDP, considering both the dynamics and electronic states, which can not be done by the previous simulation programs. Moreover, we suggested that the MgO quantum dot structure with (111) orientation covered by (001) surface has the highest stability compared to MgO(001) and MgO(011) surfaces. Finally, we recommended that our MgO(111) model is most favorable for the protecting layer in the PDP.

References

[1] K. Uetani, H. Kajiyama, A. Kato, A. Takgai, I. Tokomoto, Y. Koizumi, K. Nose, Y. Ihara, K. Onisawa, and T. Minemura, Mater. Trans. 42 (2001) 411.

[2] K. Uetani. H. Kajiyama, A. Kato, A. Takagi, T. Hori, I. Tokomoto, Y. Koizumi, K. Nose, Y. Ihara, K. Onisawa, and T. Minemura, Mater. Trans., 42 (2001) 1870.

[3] S. J. Yoon, I. Lee, and S. C. Choi, Proc. Asia Display / IDW'01 (2001) 941.

[4] A. Yamada, A. Endou, H. Takaba, K. Teraishi, S.S.C. Ammal, M. Kubo, K.G. Nakamura, M. Kitajima, and A. Miyamoto, Jpn. J. Appl. Phys., 38 (1999) 2434.

[5] H. Takaba, A. Endou, A. Yamada, M. Kubo, K. Teraishi, K.G. Nakamura, K. Ishioka, M. Kitajima, and A. Miyamoto, Jpn. J. Appl. Phys., 39 (2000) 2744.

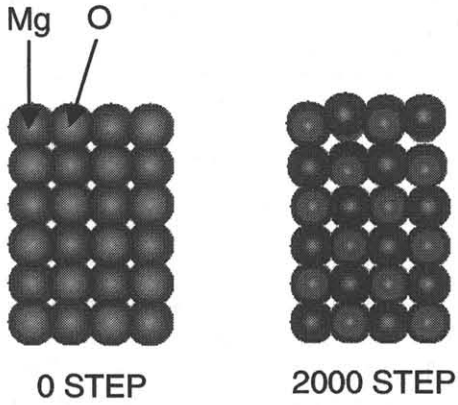

Fig. 1 Dynamic behavior of MgO(001) surface at 0.15 V/Å.

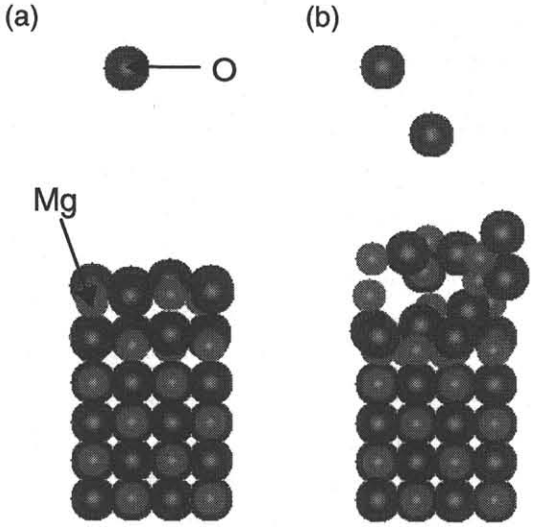

Fig. 2 Final structures of MgO(001) surface at (a) 0.20 V/Å and (b) 0.30 V/Å after the simulation.

Table 1 Effects of the orientation of the MgO surfaces and electric fields to the stability of the MgO surfaces.

	(001)	(011)	(111)
0.10 V/Å	not	not	not
0.15 V/Å	not	evap.	not
0.20 V/Å	evap.	evap.	not
0.30 V/Å	evap.	evap.	evap.